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Density functional study of cyclacene-based carbon nanotubular compounds.[1] SHINYA OKANO, Michigan State University, GLEN P. MILLER, University of New Hampshire, DAVID TOMANEK, Michigan State University — We use *ab initio* Density Functional calculations to investigate the interplay between structural and electronic properties of a new class of one-dimensional nanowires, related to carbon nanotubes. The cyclacene building blocks consist of phenyl rings, and can be viewed as the shortest segments of (n,0) zigzag nanotubes. In our study, we focus on cyclacenes with n=6-12 phenyl rings, and compare our results to infinitely large cyclacenes, corresponding to narrow graphene ribbons. The nanowires are formed by inter-connecting cyclacenes to a chain using biphenyl, tetrazine, or acetylene linkers. Depending on the nature and the orientation of the linkers, we find it possible to change the systems from narrow- to wide-gap semiconductors, and to modulate the band dispersion, suggesting the possibility of band gap engineering. We will also discuss the relevance of our results for a diameter- and chirality-selective synthesis of carbon nanotubes.

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